CHEMSTRUCT

Chemische Strukturformeln mit TEX

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Anmerkungen:

An der CYBER des EDV-Zentrums der TU Wien sind die in diesem Handbuch beschriebenen Macros im File `CHEMSTRUCT_TEX` definiert, sie werden also mit dem TEX-Befehl

```
\input chemstruct
```

verfügbar gemacht.

Die Verwendung ist sowohl in Plain TEX als auch (mit Einschränkungen) in LaTEX möglich.

Die schrägen Linien in den Strukturformeln werden aus sehr vielen Punkten zusammengesetzt. Dies kann bei manchen Driver-Programmen und Ausgabegeräten zu Speicher-Problemen führen. Bei dem an der TU Wien installierten PostScript-Driver von Nelson Beebe sind bisher *keine* solchen Probleme aufgetreten.

Das EDV-Zentrum der TU Wien dankt Herrn Dr. Ramek dafür, daß er uns seine Macros zur Verfügung gestellt hat.

H. Partl, TU Wien, 1988-11-28

Handbuch-Nummer: X14

INTRODUCTION

TEX offers excellent tools for mathematical formulae but lacks corresponding commands for most other fields of science. The purpose of this contribution is to present the macro `\structure` and a set of secondary macros, which allow an easy (but not unlimited) generation of the structural formulas used in chemistry. Portability should be guaranteed, since these macros are designed to work in the plain TEX environment. No additional font tables are required.

The following sections explain the rules for usage and the limitations of `\structure` and all its secondary macros. As examples, the instructions used to generate the figures of this paper are listed in an appendix; readers are encouraged to crosscheck this appendix with the figures.

THE CONNECTION TO PLAIN TEX

`\structure` will generate a hbox, which can be used either immediately or saved by `\newbox\name \setbox\name=\structure{...}` for a later `\copy\name` or `\box\name`, if the same structural formula is needed more than once.

The baseline of the hbox generated is identical with the baseline of the first atom or bond entry in the argument of `\structure`, height and depth depend on the subsequent entries. The width of this hbox is adjusted by `\structure` in processing the argument twice: once, without printing, to determine the amount of backspacing produced by all entries and a second time, after proper kerning, to actually do the print. This two step process combines correct positioning with the possibility to commence the structural formula definition at any atom. For testing purposes, or when starting with the leftmost atom, the first pass can and should be suppressed by issuing the command `\nopositioncheck` as the first entry in the argument of `\structure`.

The secondary macros, which actually generate the formulas, are described in the following sections. They should only be used inside the argument of `\structure`; an outside use may cause severe troubles by changing registers, dimensions, and boxes. Additional macros are used by the secondary macros; the names of these further macros contain one uppercase vowel somewhere in the middle to avoid inference with other user defined macros.

ATOMS AND BONDS

Atoms are depicted in structural formulas by their chemical symbol. It is easy to generate all possible symbols with TEX's font tables at hand, quite contrary to their proper positioning. Latter is achieved by the `\atom` macro with the chemical symbol as the argument. "Invisible" atoms, i. e. empty boxes with correct height, depth, and width for a given chemical symbol, can be generated by the `\phantatom` macro with that symbol as the argument.

Chemical bonding is symbolized in structural formulas by lines connecting the atoms. These lines also bear additional information: electronic properties (single, double, or triple bonding), nuclear geometry (esp. linear vs. non-linear), and steric arrangement (in plane, above or below the plane). The bond macros available in `\structure` are named according to a system which combines all these informations in a simple way: the direction of the bond (given in "geographic" terms: `n`, `nne`, `ne`, `ene`, `e`, `ese`, `se`, `sse`, `s`, `ssw`, `sw`, `wsw`, `w`, `wnw`, `nw`, `nnw`) is followed either by `single`, `double`, `triple`, or `phantom` (i. e. invisible) for in-plane bonds or, for out-of-plane bonds, by `below`, `above`, or `evoba` (i. e. a bond from above-plane down to in-plane). Directions for in-plane and out-of-plane bonds are not compatible: `\nnwsingle`, `\nnwdouble`, `\nnwtriple`, and `\nnwphantom` have one common direction; `\nnwabove`, `\nnwevoba`, and `\nnwbelow` have another common direction, which is slightly different from that of the `\nnwsingle`-group. Not all combinations of direction and bond type are defined; fig. 1 shows all available visible bonds with their direction codes. Bond macros have no argument.

For correct positioning, the last entry of `\structure` is expected to be either `\atom` or `\phantatom`. (The first entry may be an atom or a bond.)

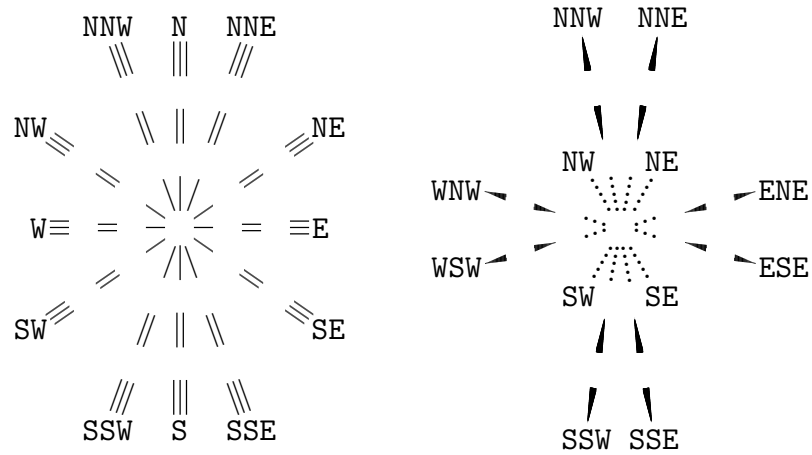

Fig. 1: All available in-plane and out-of-plane bonds.

RINGS

The in-plane bonds allow a variety of ring shapes; fig. 2 shows a sample collection. Rings built up by identical atoms will close as perfect as the ones in fig. 2 do: the $(n+1)$th atom in a n-membered ring is printed exactly at the same position as the first atom. For rings built up by different atoms, however, chances are high for a mismatch due to different widths of the atom symbols. In such cases it is adviseable to begin a ring with an `\atom` and to end it with a `\phantatom`.

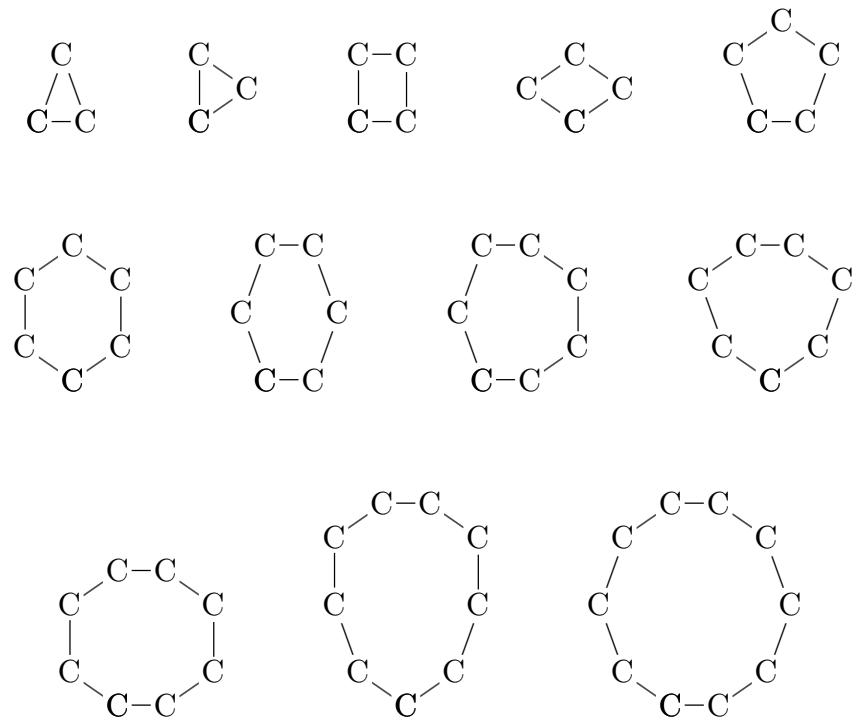

Fig. 2: Three- to tenmembered carbon rings.

Aromatic rings can be specified by generating four outmost ring atoms by `\wmostaromatatom`, `\nmostaromatatom`, `\smostaromatatom`, and `\emostaromatatom` instead of simply `\atom`. The order of these four atoms is arbitrary; they can not be made invisible though.

Unusually long single bonds, connecting atoms across a ring, can be generated by using the macros `\firstbicycloatom` and `\secondbicycloatom` instead of `\atom`. Again, these atoms are always visible. As the names indicate, the `\firstbicycloatom` must be definied

before the `\secondbicycloatom`. Nesting of such long bond definitions is impossible: a second or third bond across a ring can not be specified before completion of the previous one.

Both of these groups of macros (aromatic rings and bicyclo bonds) use the same internal registers, so they can only be used one after the other. Chemists will not regret the impossibility to define a ring as both, aromatic and bicyclic. They will, however, appreciate a facility to nest bridging bonds for the generation of tricyclic or polycyclic rings; the instructions used to generate fig. 3, which displays an aromatic, a bicyclic, a tricyclic, and a tetracyclic ring, show how to handle such problems.

Bicyclo bonds and the ellipses marking aromatic rings have more in common than just internal registers: they can never be predefined in a font table but have to be generated anew whenever needed by a long sequence of tiny little rule boxes. Only this method of generation makes them flexible enough to handle all possible situations (fig. 3 and 4 show how different aromatic rings may look). There is, however, a problem caused by this method of generation: it needs a large portion of TEX's memory. Pages full of aromatic rings or bicyclo bonds may require memory enlargement. (This manuscript was prepared with the standard main memory size of 58000.)

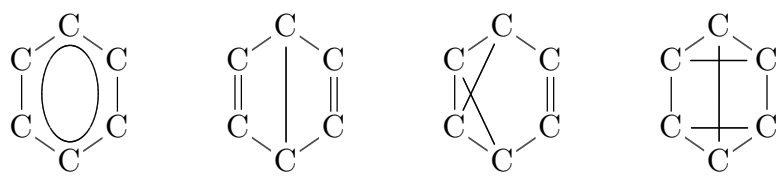

Fig. 3: Four different benzene structures.

Due to their generation by a series of rule boxes, bicyclo bonds need considerably more computer time than ordinary bonds do. Whenever possible, bridging in bicyclic rings should therefore be specified by normal bonds, as it was done in fig. 4. Bicyclo bonds can also be used to close mismatching rings (as the one shown in fig. 5 with mixed in-plane and out-of-plane bonds having slightly different lengths).

SIDE CHAINS

Side chains are generated by the `\side` macro. (In this context, a "side chain" is anything attached to the main chain by some type of bond.) The `\side` macro argument is the sequence of bonds and atoms, which define the side chain. This sequence must begin with a bond and must end with an `\atom` or `\phantatom`.

`\side` has to be called immediately after the atom, to which the side chain is bound. The definition of the main chain will be completely suspended while `\side` is processed, which is especially important for the definition of aromatic rings or bicyclo bonds: partially specified aromatic rings or bicyclo bonds will be saved when `\side` is entered and restored when `\side` is left, thus `\side` does not affect incomplete specifications of aromatic rings or bicyclo bonds at all. Furthermore, `\side` is able to generate aromatic rings or bicyclo bonds of its own, as long as all necessary specifications are part of its argument (fig. 6 was generated in this way).

Side chains often have side chains themselves. Therefore `\side` may be called from inside `\side`, the maximum nesting of side chains being 20: `\side` may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`, which in turn may be called from an outer `\side`. (Nesting side chains to that extent might need an enlargement of TEX's input stack size; this manuscript was prepared with the standard input stack size of 200.)

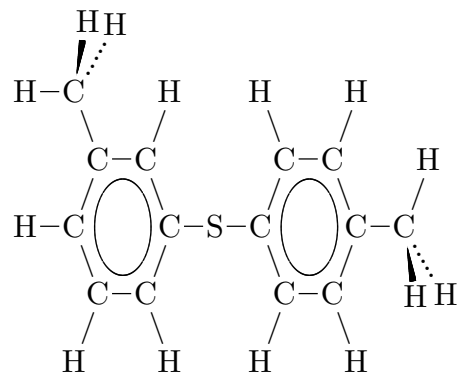

Fig. 6: 3,4'-Ditolylsulfide

LARGER STRUCTURES

Structural formulas of considerable complexity can be generated with the macros discussed so far. Fig. 7–10 show a number of examples. These examples have also been included to point out the following details: `\sseabove` goes with `\sebelow` in fig. 6 and with `\sswbelow` in fig. 7 (as does `\nneabove` with `\nebelow` and `\nnebelow` etc.);

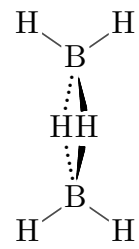

Fig. 7: Diborane

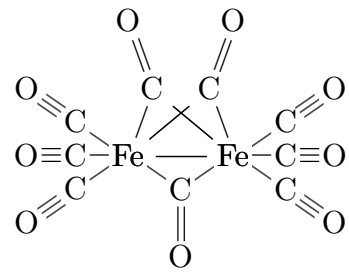

Fig. 8: Tri-μ-carbonyl-bis(tricarbonyliron)

bonds below the plane may also be used to symbolize weak bonds (fig. 9); an active character (˜) can be used to compensate additional superscripts or subscripts (fig. 9);

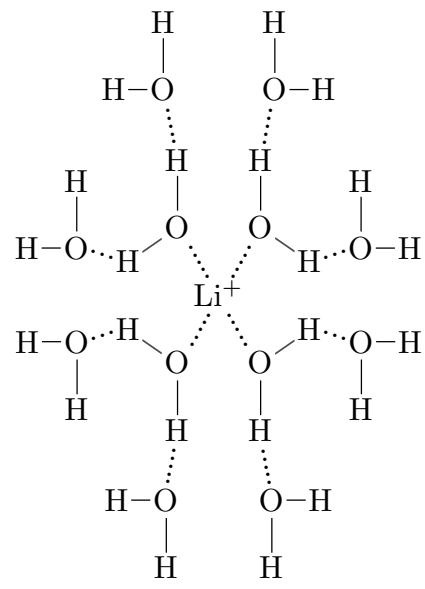

Fig. 9: A lithium cation surrounded by two hydration spheres

the choice of baseline, eventually with the help of invisible atoms and bonds, may be essential when structural formulas are combined with text or other symbols (fig. 10).

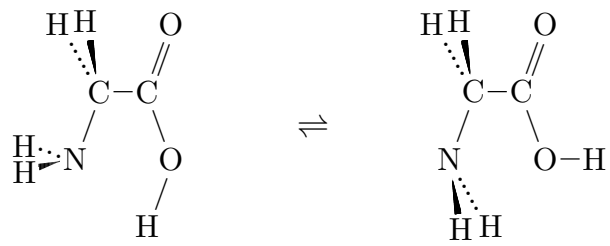

Fig. 10: Two conformeres of neutral glycine in equilibrium

For even larger structures like the ones shown in fig. 11 and 12 the four macros `\wpin`, `\epin`, `\spin`, and `\npin` may be of interest: these macros generate side chains, which are attached to the main chain without an explicitly drawn bond. Fig. 11 also illustrates the multiple use of substructures saved in boxes.

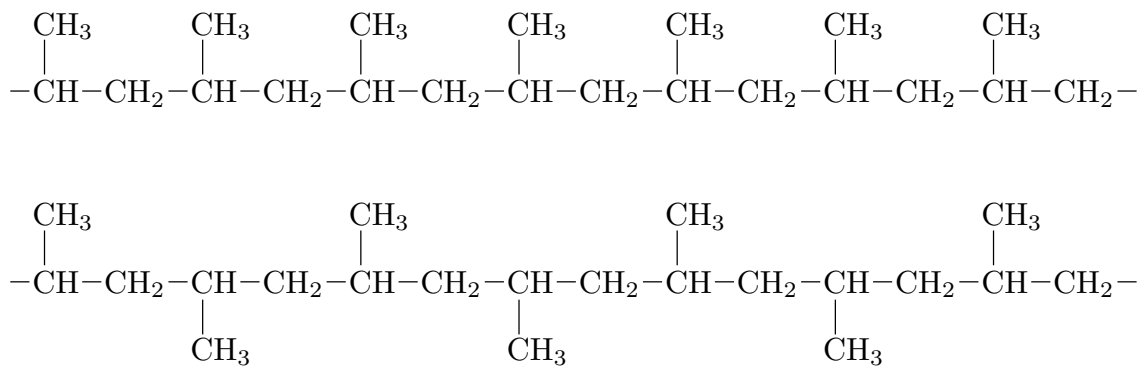

Fig. 11: Isotactic and syndiotactic polypropylene

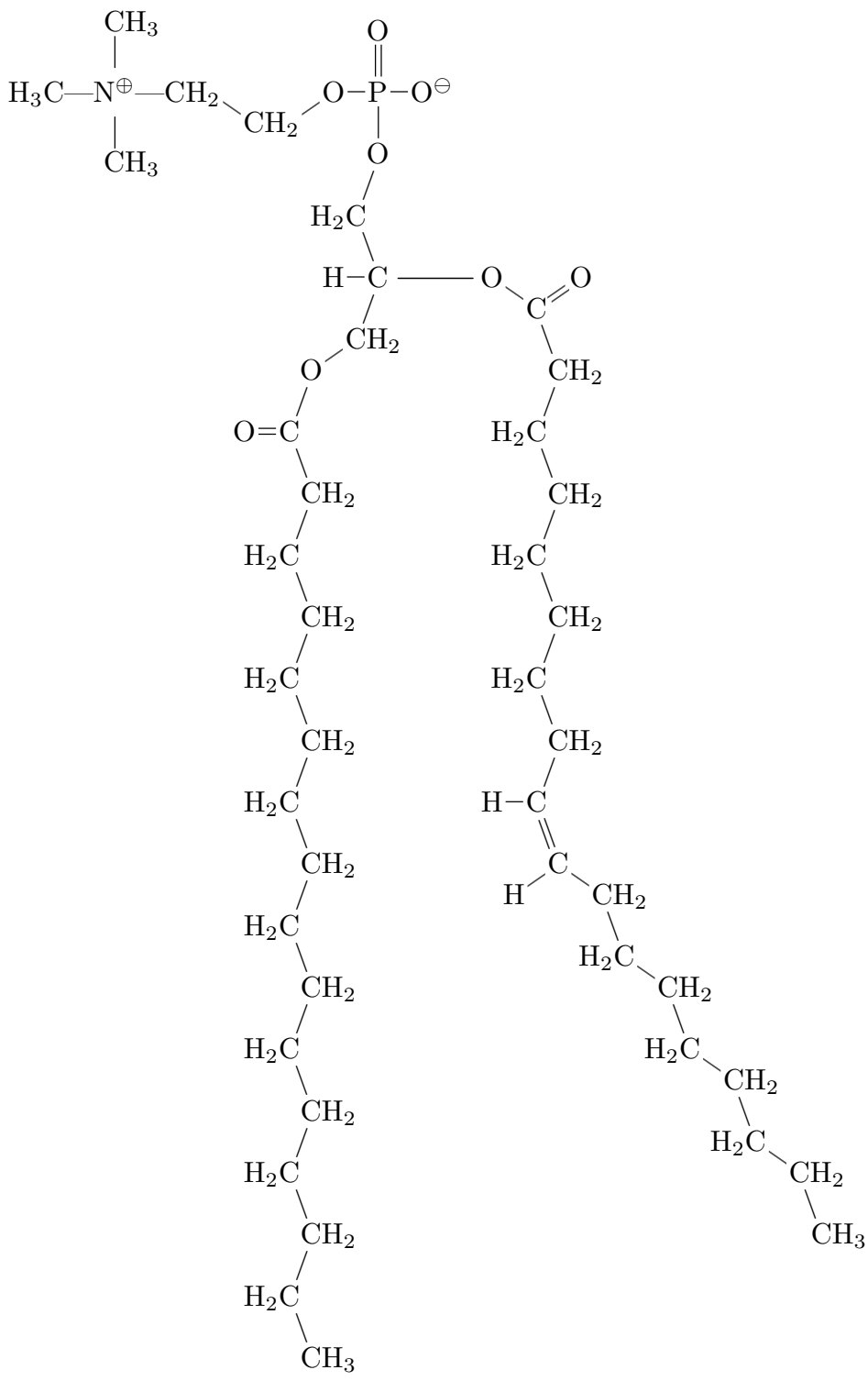

Fig. 12: 1-Palmitoyl-2-oleoyl-3-sn-glycerophosphocholin

APPENDIX

Here the instructions used to generate the figures in this paper are given.

Fig. 1:

```
%SUBJECT: File CHEMF1.TEX
\vbox{
\centerline{
\structure{\phantatom{C}
% The \phantatom just processed defines the central empty spot, from
% which all the bonds spray out; each one of the following \side{...}
% commands will generate one direction. The rules for \side are explained
% later in this paper.
\side{\wsingle\phantatom{C}\wdouble\phantatom{C}\wtriple\atom{\tt W}}
\side{\esingle\phantatom{C}\edouble\phantatom{C}\etriple\atom{\tt E}}
\side{\ssingle\phantatom{C}\sdouble\phantatom{C}\striple\atom{\tt S}}
\side{\nsingle\phantatom{C}\ndouble\phantatom{C}\ntriple\atom{\tt N}}
\side{\swsingle\phantatom{C}\swdouble\phantatom{C}\swtriple\atom{\tt SW}}
\side{\sesingle\phantatom{C}\sedouble\phantatom{C}\setriple\atom{\tt SE}}
\side{\nesingle\phantatom{C}\nedouble\phantatom{C}\netriple\atom{\tt NE}}
\side{\nwsingle\phantatom{C}\nwdouble\phantatom{C}\nwtriple\atom{\tt NW}}
\side{\nnwsingle\phantatom{C}\nnwdouble\phantatom{C}\nnwtriple
\atom{\tt NNW}}
\side{\nnesingle\phantatom{C}\nnedouble\phantatom{C}\nnetriple
\atom{\tt NNE}}
\side{\ssesingle\phantatom{C}\ssedouble\phantatom{C}\ssetriple
\atom{\tt SSE}}
\side{\sswsingle\phantatom{C}\sswdouble\phantatom{C}\sswtriple
\atom{\tt SSW}}
}
\hskip 1truecm
\structure{\phantatom{C}
\side{\wnwbelow\phantatom{C}\wnwabove\phantatom{C}\wnwevoba
\atom{\tt WNW}}
\side{\enebelow\phantatom{C}\eneabove\phantatom{C}\eneevoba
\atom{\tt ENE}}
\side{\wswbelow\phantatom{C}\wswabove\phantatom{C}\wswevoba
\atom{\tt WSW}}
\side{\esebelow\phantatom{C}\eseabove\phantatom{C}\eseevoba
\atom{\tt ESE}}
\side{\swbelow\atom{\tt SW}}
\side{\sebelow\atom{\tt SE}}
\side{\nebelow\atom{\tt NE}}
\side{\nwbelow\atom{\tt NW}}
```

```
\side{\nnwbelow\phantatom{C}\nnwabove\phantatom{C}\nnwevoba
\atom{\tt NNW}}
\side{\nnebelow\phantatom{C}\nneabove\phantatom{C}\nneevoba
\atom{\tt NNE}}
\side{\ssebelow\phantatom{C}\sseabove\phantatom{C}\sseevoba
\atom{\tt SSE}}
\side{\sswbelow\phantatom{C}\sswabove\phantatom{C}\sswevoba
\atom{\tt SSW}}
}
}
\vskip 1truecm
\centerline{\it Fig.~1: All available in-plane and out-of-plane bonds.}
}
```

Fig. 2:

```
%SUBJECT: File CHEMF2.TEX
\vbox{
\centerline{
\structure{\nopositioncheck\atom{C}\esingle\atom{C}\nnwsingle
\atom{C}\sswsingle\atom{C}}
\hskip 1truecm
\structure{\nopositioncheck\atom{C}\nsingle\atom{C}\sesingle\atom{C}
\swsingle\atom{C}}
\hskip 1truecm
\structure{\nopositioncheck\atom{C}\nsingle\atom{C}\esingle\atom{C}
\ssingle\atom{C}\wsingle\atom{C}}
\hskip 1truecm
\structure{\atom{C}\nwsingle\atom{C}\nesingle\atom{C}\sesingle
\atom{C}\swsingle\atom{C}}
\hskip 1truecm
\structure{\atom{C}\nnwsingle\atom{C}\nesingle\atom{C}\sesingle
\atom{C}\sswsingle\atom{C}\wsingle\atom{C}}
}
\vskip 1truecm
\centerline{
\structure{\atom{C}\nwsingle\atom{C}\nsingle\atom{C}\nesingle\atom{C}
\sesingle\atom{C}\ssingle\atom{C}\swsingle\atom{C}}
\hskip 1truecm
\structure{\atom{C}\nnwsingle\atom{C}\nnesingle\atom{C}\esingle
\atom{C}\ssesingle\atom{C}\sswsingle\atom{C}\wsingle\atom{C}}
\hskip 1truecm
\structure{\atom{C}\nnwsingle\atom{C}\nnesingle\atom{C}\esingle
\atom{C}\sesingle\atom{C}\ssingle\atom{C}\swsingle\atom{C}\wsingle
```

```
\atom{C}}
\hskip 1truecm
\structure{\atom{C}\nwsingle\atom{C}\nnwsingle\atom{C}\nesingle
\atom{C}\esingle\atom{C}\sesingle\atom{C}\sswsingle\atom{C}\swsingle
\atom{C}}
}
\vskip 1truecm
\centerline{
\structure{\atom{C}\nwsingle\atom{C}\nsingle\atom{C}\nesingle\atom{C}
\esingle\atom{C}\sesingle\atom{C}\ssingle\atom{C}\swsingle\atom{C}
\wsingle\atom{C}}
\hskip 1truecm
\structure{\atom{C}\nwsingle\atom{C}\nnwsingle\atom{C}\nsingle
\atom{C}\nesingle\atom{C}\esingle\atom{C}\sesingle\atom{C}\ssingle
\atom{C}\sswsingle\atom{C}\swsingle\atom{C}}
\hskip 1truecm
\structure{\atom{C}\nwsingle\atom{C}\nnwsingle\atom{C}\nnesingle
\atom{C}\nesingle\atom{C}\esingle\atom{C}\sesingle\atom{C}\ssesingle
\atom{C}\sswsingle\atom{C}\swsingle\atom{C}\wsingle\atom{C}}
}
\vskip 1truecm
\centerline{\it Fig.~2: Three- to tenmembered carbon rings.}
}
```

Fig. 3:

```
%SUBJECT: File CHEMF3.TEX
\vbox{
\centerline{
\structure{\nopositioncheck\wmostaromatatom{C}\nsingle\atom{C}
\nesingle\nmostaromatatom{C}\sesingle\emostaromatatom{C}\ssingle
\atom{C}\swsingle\smostaromatatom{C}\nwsingle\phantatom{C}}
\hskip 1truecm
\structure{\nopositioncheck\atom{C}\ndouble\atom{C}\nesingle
\firstbicycloatom{C}\sesingle\atom{C}\sdouble\atom{C}\swsingle
\secondbicycloatom{C}\nwsingle\phantatom{C}}
\hskip 1truecm
\structure{\nopositioncheck\firstbicycloatom{C}\nsingle
\phantatom{C}\nesingle\secondbicycloatom{C}\swphantom
\firstbicycloatom{C}\nephantom\phantatom{C}\sesingle\atom{C}\sdouble
\atom{C}\swsingle\secondbicycloatom{C}\nwsingle\phantatom{C}}
\hskip 1truecm
\structure{\nopositioncheck\firstbicycloatom{C}\sesingle
\phantatom{C}\nephantom\secondbicycloatom{C}\swsingle
```

```
\firstbicycloatom{C}\nephantom\phantatom{C}\nsingle\phantatom{C}
\nwsingle\secondbicycloatom{C}\sephantom\firstbicycloatom{C}
\nwphantom\phantatom{C}\swsingle\secondbicycloatom{C}\ssingle
\phantatom{C}}
}
\vskip 1truecm
\centerline{\it Fig.~3: Four different benzene structures.}
}
```

Fig. 4 & 5:

```
%SUBJECT: File CHEMF45.TEX
\hbox{\vbox{
\hbox to 0.5\hsize{\hss
\structure{\emostaromatatom{C}\swsingle\smostaromatatom{C}\wsingle
\atom{C}\nnwsingle\wmostaromatatom{C}\nnesingle\nmostaromatatom{C}
\esingle\atom{C}\sesingle\wmostaromatatom{C}\nesingle
\nmostaromatatom{C}\ssesingle\emostaromatatom{C}\sswsingle
\smostaromatatom{C}\nwsingle\phantatom{C}\nsingle\phantatom{C}}
\hss}
\vskip 1truecm
\hbox to 0.5\hsize{\hss\it Fig.~4: The azulene ring system.\hss}
}\vbox{
\hbox to 0.5\hsize{\hss
\structure{\firstbicycloatom{C}\nnwsingle\atom{C}\eneabove\atom{C}
\eseevoba\atom{C}\sswsingle\secondbicycloatom{C}}
\hss}
\vskip 1truecm
\hbox to 0.5\hsize{\hss\it Fig.~5: The envelope form of cyclopentane.\hss}
}}
```

Fig. 6:

```
%SUBJECT: File CHEMF6.TEX
\vbox{
\centerline{
\structure{\nopositioncheck\atom{H}\esingle\wmostaromatatom{C}
\nnesingle\nmostaromatatom{C}
\side{\nnwsingle\atom{C}\side{\nneabove\atom{H}}
\side{\nebelow\atom{H}}\wsingle\atom{H}}
\esingle\atom{C}\side{\nnesingle\atom{H}}\ssesingle\emostaromatatom{C}
\side{\esingle\atom{S}\esingle\wmostaromatatom{C}\nnesingle\atom{C}
\side{\nnwsingle\atom{H}}\esingle\nmostaromatatom{C}\side{\nnesingle
\atom{H}}\ssesingle\emostaromatatom{C}\side{\esingle\atom{C}
\side{\sseabove\atom{H}}\side{\sebelow\atom{H}}\nnesingle\atom{H}}
```

```
\sswsingle\smostaromatatom{C}\side{\ssesingle\atom{H}}\wsingle
\atom{C}\side{\sswsingle\atom{H}}\nnwsingle\phantatom{C}}
\sswsingle\atom{C}\side{\ssesingle\atom{H}}\wsingle
\smostaromatatom{C}\side{\sswsingle\atom{H}}\nnwsingle\phantatom{C}}
}
\vskip 1truecm
\centerline{\it Fig.~6: 3,4'-Ditolylsulfide}
}
```

Fig. 7:

```
%SUBJECT: File CHEMF7.TEX
\vbox{
\centerline{
\structure{\nopositioncheck\atom{H}\sesingle
\atom{B}\side{\nesingle\atom{H}}
\sseabove\atom{H}\sswevoba\atom{B}
\side{\nnwbelow\atom{H}\nnebelow\phantatom{B}}
\side{\swsingle\atom{H}}\sesingle\atom{H}}
}
\vskip 1truecm
\centerline{\it Fig.~7: Diborane}
}
```

Fig. 8:

```
%SUBJECT: File CHEMF8.TEX
\vbox{
\centerline{\structure{\nopositioncheck
\atom{O}\etriple\atom{C}\esingle\firstbicycloatom{Fe}
\side{\nwsingle\atom{C}\nwtriple\atom{O}}
\side{\swsingle\atom{C}\swtriple\atom{O}}
\sesingle\atom{C}\side{\sdouble\atom{O}}\nesingle\phantatom{Fe}
\side{\esingle\atom{C}\etriple\atom{O}}
\side{\sesingle\atom{C}\setriple\atom{O}}
\side{\nesingle\atom{C}\netriple\atom{O}}
\nnwsingle\secondbicycloatom{C}\side{\nnedouble\atom{O}}
\ssephantom\firstbicycloatom{Fe}\swphantom\phantatom{C}\nwphantom
\phantatom{Fe}\nnesingle\secondbicycloatom{C}\side{\nnwdouble\atom{O}}
\sswphantom\firstbicycloatom{Fe}\sephantom\phantatom{C}\nephantom
\secondbicycloatom{Fe}}}
\vskip 1truecm
\centerline{\it Fig.~8: Tri-$\mu$-carbonyl-bis(tricarbonyliron)}
}
```

Fig. 9:

```
%SUBJECT: File CHEMF9.TEX
\vbox{
\centerline{
\structure{\atom{~~Li$^+$}
\side{\nwbelow\atom{O}
\side{\nsingle\atom{H}\nnwbelow\atom{O}\side{\wsingle\atom{H}}
\nsingle\atom{H}}\swsingle\atom{H}\wnwbelow\atom{O}
\side{\wsingle\atom{H}}\nsingle\atom{H}}
\side{\nebelow\atom{O}
\side{\nsingle\atom{H}\nnebelow\atom{O}\side{\esingle\atom{H}}
\nsingle\atom{H}}\sesingle\atom{H}\enebelow\atom{O}
\side{\esingle\atom{H}}\nsingle\atom{H}}
\side{\swbelow\atom{O}
\side{\ssingle\atom{H}\sswbelow\atom{O}\side{\wsingle\atom{H}}
\ssingle\atom{H}}\nwsingle\atom{H}\wswbelow\atom{O}
\side{\wsingle\atom{H}}\ssingle\atom{H}}
\side{\sebelow\atom{O}
\side{\ssingle\atom{H}\ssebelow\atom{O}\side{\esingle\atom{H}}
\ssingle\atom{H}}\nesingle\atom{H}\esebelow\atom{O}
\side{\esingle\atom{H}}\ssingle\atom{H}}}
}
\vskip 1truecm
\centerline
{\it Fig.~9: A lithium cation surrounded by two hydration spheres}
}
```

Fig. 10:

```
%SUBJECT: File CHEMF10.TEX
\vbox{
\centerline{
\structure{\nopositioncheck\phantatom{H}\sephantom\atom{N}
\side{\wswabove\atom{H}}\side{\wnwbelow\atom{H}}\nnesingle\atom{C}
\side{\nnwabove\atom{H}}\side{\nwbelow\atom{H}}\esingle\atom{C}
\side{\nnedouble\atom{O}}\ssesingle\atom{O}\sswsingle\atom{H}}
\hskip 1cm{$\rightleftharpoons$}\hskip 1cm
\structure{\phantatom{H}\swphantom\atom{N}\side{\sseabove\atom{H}}
\side{\sebelow\atom{H}}\nnesingle\atom{C}\side{\nnwabove\atom{H}}
\side{\nwbelow\atom{H}}\esingle\atom{C}\side{\nnedouble\atom{O}}
\ssesingle\atom{O}\esingle\atom{H}}
}
\vskip 1truecm
\centerline{\it
```

```
Fig.~10: Two conformeres of neutral glycine in equilibrium}
}
```

Fig. 11:

```
%SUBJECT: File CHEMF11.TEX
\newbox\monomera\setbox\monomera=
\structure{\nopositioncheck\esingle\atom{C}
\side{\nsingle\atom{C}\epin{H$_3$}}
\atom{H}\esingle\atom{CH$_2$}}
\newbox\monomerb\setbox\monomerb=
\structure{\nopositioncheck\esingle\atom{C}
\side{\ssingle\atom{C}\epin{H$_3$}}
\atom{H}\esingle\atom{CH$_2$}}
\newbox\monomere\setbox\monomere=
\structure{\nopositioncheck\esingle\atom{C}
\side{\nsingle\atom{C}\epin{H$_3$}}
\atom{H}\esingle\atom{CH$_2$}\esingle\phantatom{}}
\vbox{
\centerline{\copy\monomera\copy\monomera\copy\monomera\copy\monomera
\copy\monomera\copy\monomera\copy\monomere}
\vskip 1truecm
\centerline{\copy\monomera\copy\monomerb\copy\monomera\copy\monomerb
\copy\monomera\copy\monomerb\copy\monomere}
\vskip 1truecm
\centerline{\it Fig.~11: Isotactic and syndiotactic polypropylene}
}
```

Fig. 12:

```
%SUBJECT: File CHEMF12.TEX
\vbox{
\centerline{\structure{
\atom{C}\epin{H$_3$}\nnwsingle\atom{C}\wpin{H$_2$}
\nnesingle\atom{C}\epin{H$_2$}\nnwsingle\atom{C}\wpin{H$_2$}
\nnesingle\atom{C}\epin{H$_2$}\nnwsingle\atom{C}\wpin{H$_2$}
\nnesingle\atom{C}\epin{H$_2$}\nnwsingle\atom{C}\wpin{H$_2$}
\nnesingle\atom{C}\epin{H$_2$}\nnwsingle\atom{C}\wpin{H$_2$}
\nnesingle\atom{C}\epin{H$_2$}\nnwsingle\atom{C}\wpin{H$_2$}
\nnesingle\atom{C}\epin{H$_2$}\nnwsingle\atom{C}\wpin{H$_2$}
\nnesingle\atom{C}\epin{H$_2$}\nnwsingle\atom{C}\side{\wdouble\atom{O}}
\nnesingle\atom{O}\nesingle\atom{C}\epin{H$_2$}
\nnesingle\firstbicycloatom{C}\side{\wsingle\atom{H}}
\nnwsingle\atom{C}\wpin{H$_2$}\nnesingle\atom{O}
\side{\nsingle\atom{P}\side{\esingle\atom{O$^\ominus$}}
```

```
\side{\ndouble\atom{O}}
\side{\wsingle\atom{O}\swsingle\atom{CH$_2$}\nwsingle
\atom{~~H$_3$C---N$^\oplus$---CH$_2$}
\side{\nsingle\atom{C}\epin{H$_3$}}\side{\ssingle\atom{C}\epin{H$_3$}}}}
\ephantom\phantatom{OOO}\ephantom\ssephantom\phantatom{O}\sswphantom
\secondbicycloatom{O}\sesingle\atom{C}\side{\nedouble\atom{O}}
\ssesingle\atom{C}\epin{H$_2$}\sswsingle\atom{C}\wpin{H$_2$}
\ssesingle\atom{C}\epin{H$_2$}\sswsingle\atom{C}\wpin{H$_2$}
\ssesingle\atom{C}\epin{H$_2$}\sswsingle\atom{C}\wpin{H$_2$}
\ssesingle\atom{C}\epin{H$_2$}\sswsingle\atom{C}\side{\wsingle\atom{H}}
\ssedouble\atom{C}\side{\swsingle\atom{H}}
\sesingle\atom{C}\epin{H$_2$}\ssesingle\atom{C}\wpin{H$_2$}
\sesingle\atom{C}\epin{H$_2$}\ssesingle\atom{C}\wpin{H$_2$}
\sesingle\atom{C}\epin{H$_2$}\ssesingle\atom{C}\wpin{H$_2$}
\sesingle\atom{C}\epin{H$_2$}\ssesingle\atom{C}\epin{H$_3$}}}
\vskip 1truecm
\centerline{\it Fig.~12:
1-Palmitoyl-2-oleoyl-3-\underbar{sn}-glycerophosphocholin}
}
```